NATIONAL WATER RESEARCH INSTITUTE

INSTITUT NATIONAL de RECHERCHE sur les EAUX

EXPRES: AN EXPERT SYSTEM FOR ASSESSING THE FATE OF PESTICIDES IN THE SUBSURFACE

J.P. Mutch and A.S. Crowe

NWRI CONTRIBUTION 90-98

RRB 90-67

EXPRES: AN EXPERT SYSTEM FOR ASSESSING THE FATE OF PESTICIDES IN THE SUBSURFACE

PHASE FOUR REPORT: VERIFICATION OF PESTICIDE MODELS INCORPORATED IN EXPRES

by

J.P. Mutch and A.S. Crowe

Rivers Research Branch
National Water Research Institute
Canada Centre for Inland Waters
Burlington, Ontario, L7R 4A6

NOVEMBER 1990
NWRI Contribution #90-98

MANAGEMENT PERSPECTIVE

The Pesticide Division of the Commercial Chemicals Branch, Environment Canada, is required to assess the environmental hazards associated with a pesticide and its transformation products before it is approved for public use. One specific concern of the Pesticide Division is the potential for a pesticide to contaminate shallow groundwater resources. Although a number of models currently exist that can predict the transport and transformation of pesticides in the subsurface, generally, regulatory personnel do not have the expertise required to accurately utilize these models. The Groundwater Contamination Project, NWRI, was approached by the Pesticide Division to develop an expert system that can be used to aid in the assessment of the potential for groundwater contamination by pesticides. In addition, this expert system can be used for the identification of agricultural development which may or may not be sustainable.

This report discusses work completed in Phase 4 of a two year program currently being undertaken by the Groundwater Contamination Project to develop the expert system. Specifically, the report describes the verification of the modified versions of the two pesticide models (LEACHM and PRZM) incorporated in the EXPRES expert system, and the testing of the dialogue portion of the expert system and the interaction between the expert system and the pesticide models. The tests described here in, were preformed to ensure that the data files created by the EXPRES expert system are being read and executed correctly by the modified versions of the pesticide models. All verification tests performed indicate that the two pesticide models in the expert system are operating correctly.

PERSPECTIVES DE GESTION

La Division des pesticides de la Direction des produits chimiques commerciaux d'Environnement Canada est tenue d'évaluer les risques pour l'environnement que constituent un pesticide et ses produits de transformation, avant d'autoriser sa commercialisation. L'un des problèmes auxquels est confrontée la Division des pesticides : le risque de contamination d'eaux souterraines peu profondes par un pesticide. Bien qu'il existe actuellement un certain nombre de modèles qui peuvent prédire les processus de transport et de transformation des pesticides sous la surface du sol, le personnel chargé de la réglementation n'a généralement pas la compétence requise pour utiliser adéquatement ces modèles. La Division des pesticides s'est intéressée au projet relatif à la contamination des eaux souterraines de l'INRE en vue d'élaborer un système-expert, qui faciliterait l'évaluation de la contamination des eaux souterraines par les pesticides. De plus, ce système-expert pourrait être utilisé pour déterminer dans quelle mesure tel ou tel développement agricole est ou n'est pas une source de risques.

Le présent rapport examine les travaux terminés dans la phase 4 du programme de deux ans actuellement en cours dans le cadre du projet mentionné ci-dessus et qui visaient l'élaboration du système-expert. Plus précisément, le rapport décrit : la vérification des versions modifiées des deux modèles de pesticides (LEACHM et PRZM) incorporés dans le système-expert EXPRES; les essais de la portion dialogue du système-expert; l'interaction entre le système-expert et le modèle de pesticide. Les essais décrits ici ont été effectués pour vérifier que les fichiers de données créés par le système-expert EXPRES sont lus et exécutés correctement par les versions modifiées des modèles de pesticides. Tous les essais de vérification effectués montrent que les deux modèles de pesticides dans le système-expert fonctionnent correctement.

ABSTRACT

The EXPRES expert system is being developed to aid regulatory personnel in their assessment of the potential for pesticides to contaminate the soil and shallow groundwater environment. The expert system, known as EXPRES (EXpert system for Pesticide Regulatory Evaluation Simulations), consists of two existing numerical models that are used to simulate the fate of pesticides in the unsaturated zone, coupled with a knowledge-based system that guides the user through the choice of all the necessary information for characterizing the physical, climatic, hydrogeological, pedological and agricultural setting of typical agricultural regions across Canada, as required by the pesticide models.

This report describes the verification of the modified versions of the two pesticide models (LEACHM and PRZM), and their interaction with the EXPRES expert system. The report briefly reviews the modifications made to the two pesticide models and describes tests that were conducted to verify the modified versions of the two pesticide models. Because both LEACHM and PRZM are widely used, and have been tested by others (Carsel et al., 1984;1985, Jones, 1985;1986, Jones et al., 1986, Wagenet and Hutson, 1986;1987 and Pennell et al., 1989); the verification tests simply ensure that the modified versions of the two pesticide models within EXPRES correctly simulate the physical and chemical processes found in nature, and that all mathematical operations within the two models are correct.

The processes added to the LEACHM model(runoff and erosion, snowmelt, and pan evaporation estimation) are similar to process originally incorporated in the PRZM model. Hence, the modifications made to the LEACHM model were verified by comparing the results produced with corresponding results produced by the original PRZM model.

The verification tests performed were successful and the modified versions of the two pesticide models are operating correctly within the EXPRES expert system.

RÉSUMÉ

Le système-expert EXPRES est destiné à aider le personnel chargé de la réglementation lors de l'évaluation des risques de contamination du sol et des eaux souterraines peu profondes par les pesticides. Le système-expert, appelé EXPRES ("EXpert system for Pesticide Regulatory Evaluation Simulations"), est constitué de deux modèles numériques existants, qui sont utilisés pour simuler le devenir des pesticides dans la zone insaturée, ces modèles étant associés à un système basé sur les connaissances, qui guide l'utilisateur à travers le choix de toute l'information nécessaire pour caractériser la situation physique, climatique, hydrogéologique, pédologique et agricole de régions rurales typiques du Canada, selon les exigences dictées par les modèles de pesticides.

Le présent rapport décrit la vérification des versions modifiées des deux modèles de pesticides (LEACHM et PRZM), et leur interaction avec le système-expert EXPRES. Le rapport examine brièvement les modifications apportées aux deux modèles de pesticides et décrit les essais qui ont été effectués pour vérifier les versions modifiées des deux modèles de pesticides. Étant donné que les systèmes LEACHM et PRZM sont largement utilisés et qu'ils ont déjà été vérifiés par d'autres (Carsel et al., 1984, 1985; Jones, 1985, 1986; Jones et al., 1986; Wagenet et Hutson, 1986, 1987; Pennet et al., 1989), les essais de vérification permettent simplement de s'assurer que les versions modifiées des deux modèles de pesticides à l'intérieur du système EXPRES simulent correctement les processus physiques et chimiques que l'on retrouve dans la nature, et que toutes les opérations mathématiques dans le cadre des deux modèles sont correctes.

Les processus ajoutés au modèle LEACHM (ruissellement et érosion, fonte des neiges et évaluation de l'évaporation en bac) sont semblables aux processus incorporés à l'origine au modèle PRZM. Ainsi, les modifications apportées au modèle LEACHM ont été vérifiées par étude comparative des résultats obtenue et des résultats correspondants provenant du modèle initial PRZM.

Les essais de vérification ont été couronnés de succès et les versions modifiées des deux modèles de pesticides fonctionnent correctement à l'intérieur du système-expert EXPRES.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1.0 INTRODUCTION

Several modifications were required to be made to the two pesticide models (LEACHM and PRZM) before they could be incorporated into the EXPRES expert system. In order to ensure that the modifications made to the two models did not disrupt the validity of the model predictions, and to ensure that the two models interact with the EXPRES expert system correctly, test have been conducted to verify the two models. The original versions of both PRZM and LEACHM have been tested by the model developers and others (Carsel et al., 1984;1985, Jones, 1985;1986, Jones et al., 1986, Wagenet and Hutson, 1986;1987 and Pennell et al., 1989). Thus further validation of the original versions of the models will not be attempted.

Therefore, the objective of Phase Four is to ensure that the results generated by EXPRES are both meaningful and accurate. Specifically, the verification process will ensure that:

(1) the arithmetic calculations in the models are correct;

(2) the physical and chemical processes added to the models are simulated correctly;

(3) the simulation options and dialogue format of EXPRES are read and executed correctly.

2.0 MODIFICATIONS MADE TO THE PESTICIDE MODELS

2.1 PRZM MODIFICATIONS

Only relatively minor modifications were made to the PRZM model to allow it to interact with the EXPRES expert system. The modifications made to PRZM include:

(1) reading input parameters from a common input data file created by EXPRES;

(2) modifying the echo subroutine to echo the PRZM-specific data that is read from the common input data file created by EXPRES;

(3) reading climatological data from a common meteorological data file.

A simulation of the transport and transformation of a pesticide in the unsaturated zone within EXPRES maybe undertaken with either the PRZM or LEACHM models. Both PRZM and LEACHM require input data describing the chemical characteristics of the pesticide, the hydrogeological setting of the site, farm management information and climatic data. Because much of these data are common to both models, it is more efficient for EXPRES to create a single common input data set that can be read by either model, than it is to construct individual data sets for the two models. However, the data specific to the model that is not being executed must be bypassed by the model that is being executed. Therefore, the subroutine in PRZM that reads the input data set was modified to read the only the data required by the PRZM model, skipping all data that is specific to the LEACHM model. The subroutine to echo the data read by PRZM was also modified to reflect these changes. In addition, the subroutine that reads the climatological data was also modified to extract the climatological data required by PRZM from a common meteorological file that contains climatological data for both the PRZM and LEACHM models.

2.2 LEACHM MODIFICATIONS

The modifications made to the LEACHM model were more extensive and include the following:

(1) reading input parameters from a common input data file created by EXPRES;

(2) adding an echo subroutine to echo the LEACHM-specific data that is read from the common input data file created by EXPRES;

(3) reading climatological data from a common meteorological data file;

(4) modifying the output subroutines;

(5) adding a snowmelt subroutine;

(6) adding a subroutine to estimate pan evaporation;

(7) adding a subroutine to estimate surface runoff and erosion.

For similar reasons as presented in Section 2.1 for the PRZM model, the LEACHM model was modified to read the input data from a common input data file created by EXPRES, and the climatological data from a common meteorological file. The original version of LEACHM did not have a subroutine to echo the data that were read, so a subroutine was added to echo the LEACHM-specific data read by the model.

The manner in which LEACHM reads the climatological data has been modified from, reading data only on days for which was rainfall, to reading daily climatic data, including daily mean temperatures. The switch was made to facilitate the incorporation of subroutines to calculate snowmelt and daily pan evaporation. Daily temperature values are used to accumulate and melt snow when appropriate, and to estimate daily pan evaporation values when actual measured pan evaporation data are not available.

Modifications have also been made to the model to allow LEACHM to simulate surface runoff and erosional losses of both water and pesticide. Mathematically, both processes are represented within the LEACHM model in the same manner as that used in the PRZM model. Erosional losses are determined with a modified Universal Soil Loss

Equation (MUSLE) approach (Williams and Brendt, 1977), and surface runoff is calculated with the curve number approach developed by the USDA Soil Conservation service (Haith and Loehr, 1979).

The reader is referred to the Phase 2 Report (Mutch and Crowe, 1990) for further details on the modifications made to the two models. A detailed description of the processes involved in surface runoff and erosion is presented by Mutch and Crowe (1989), and in the two references sited above.

3.0 MODEL VERIFICATION

3.1 VERIFICATION OF THE PRZM MODEL

Three tests were performed with both the modified and original versions of the PRZM model to verify that the modified version of PRZM, incorporated within the EXPRES expert system, is operating correctly. The three tests were designed to:

(1) check the recompilation of the PRZM program with the Microsoft® FORTRAN (v5.0) compiler;

(2) ensure that the modified input data set was being read correctly;

(3) ensure that the modified meteorological data file was being read correctly.

3.1.1 PRZM TEST 1 - RECOMPILATION OF THE PRZM PROGRAM

In the following discussions the modified version of the PRZM program, used within EXPRES, will be referred to as PRZMEX, while the original version of the model will continue to be referred to as PRZM. The first test was designed to verify the recompilation of both the PRZM and PRZMEX models with the Microsoft® FORTRAN compiler. The test consisted of two simulations. In the first simulation, the PRZM source code was compiled with the Microsoft® FORTRAN (v5.0) compiler, and the sample problem provided by the distributors (U.S. EPA) of the PRZM code was executed. The results produced with the Microsoft® FORTRAN (v5.0) version of PRZM were then compared to the output for the sample problem supplied with the PRZM model, which had been produced after compiling the PRZM source code with the Ryan-McFarland® FORTRAN (RMFORT v2.43) compiler. The output produced by the Microsoft® FORTRAN version of PRZM was the same as the supplied output.

For the second simulation, the PRZMEX program was compiled with the Microsoft® FORTRAN (v5.0) compiler, and the sample problem was executed. Again, the output produced with PRZMEX was compared to the output for the sample problem supplied with the PRZM model, and the results were identical.

As an additional verification test, the PRZMEX model was compiled and linked with the LAHEY® FORTRAN F77L-EM/32 (v2.01) compiler to identify if any additional errors or warning messages would be produced. There were no additional error messages, however, several additional warning messages (non FORTRAN-77 standard) were generated by the LAHEY® FORTRAN compiler. All warning messages, with the exception of "integer*2" and "include" statements, were eliminated from the PRZMEX model, without altering the resulting output from the model.

3.1.2 PRZM TEST 2 - VERIFICATION OF THE INPUT DATA SET

Eight simulations were performed in the second test. The objective of this test was to ensure that the common input data set was being read correctly by the modified input statements in the PRZMEX model, and that all the possible options available in the PRZMEX model were being read and executed correctly. Input data sets for both PRZM and PRZMEX were generated for four different scenarios, and the results of the four simulations with PRZMEX were compared with the corresponding results for the four simulations with PRZM.

For example, the PRZM and PRZMEX models has four possible options for the pesticide application method. The four are:

(1) a pesticide application to the soil surface;

(2) a pesticide application incorporated into the soil profile;

(3) a foliar pesticide application with a linear washoff representation;

(4) a foliar pesticide application with an exponential washoff representation.

Four pairs of input data sets (four for PRZM, and four for PRZMEX) were generated with the pesticide being applied in a different manner in each pair, thereby testing the four possible options shown above. After executing each pair, the results produced by PRZMEX were compared to the results produced with PRZM to ensure that the options had been read and executed correctly, and that the modifications did not change the results of the model.

At the same time, all other options available in the PRZM and PRZMEX models were tested in the eight simulations performed for this test. Table 1 displays the pertinent values of the model parameters used in this test. In all cases, results produced by the PRZMEX model were the same as those produced by the PRZM model. Therefore, it can be concluded that the PRZMEX version of the model correctly reads and executes the data contained in the common data file generated by EXPRES.

3.1.3 PRZM TEST 3 - VERIFICATION OF THE METEOROLOGICAL DATA

In the third test performed, the meteorological data files for the Charlottetown CDA weather station (Climatological Services Division, 1990) were tested for accuracy and errors in format. The meteorological files contain daily values for precipitation, pan evaporation, temperature and an arbitrary value for the rate of precipitation. Six simulations were performed in this test (three with PRZMEX, and three with PRZM). In the first pair of simulations, the original meteorological file provided by the distributors of the model was tested with both PRZM and PRZMEX to ensure that the modified routine in PRZMEX read the meteorological data correctly and produced accurate results. Two sets of meteorological data are required by EXPRES to test typical climatic conditions at a site within a given agricultural zone. The data contained in these files are, twenty years of actual climatic data (Jan. 1, 1970 - July 31, 1989), and one-year of daily median values for the meteorological parameters over the twenty year period.

In the second and third simulation pairs, the actual and median meteorological data files that had been compiled for the Charlottetown CDA weather station were used. No errors were detected in reading these two data files, and in all three pairs of simulations, the results produced by PRZMEX were identical to the results from PRZM. Therefore, the modified version of the PRZM model, PRZMEX, correctly reads the meteorological data.

Table 1. Model parameter data for the PRZM verification tests.

PRZM VERIFICATION				
	SIMULATION 1	SIMULATION 2	SIMULATION 3	SIMULATION 4
FILE NAME	PTEST001	PTEST002	PTEST003	PTEST004
STARTING DATE	010174	010170	010180	010173
ENDING DATE	311276	310789	311280	311277
PESTICIDE	DUMMY	SULFOXIDE	SULFONE	DUMMY
SOLUBILITY (mg/L)	6000	28000	7800	6000
K_{oc} VALUE (L/kg)	80	1.0	1.0	1.0
DEPTH OF INCORP. (cm)	0.0	10.0	0.0	0.0
APPLICATION METHOD	SOIL	SOIL	LINEAR	EXPONENT.
D.K. RATE (FOLIAGE)	0.0693	0.0693	0.0693	0.0693
FOLIAR EXTRACTION	0.10	0.1	0.1	0.10
FILTRATION PARAMETER	2.80	2.80	2.80	2.80
DEGRAD. RATE (DAY-1)	0.0100	0.00693	0.00693	0.00693
FILES GENERATED	ALL	ALL	ALL	ALL
OUTPUT TIME STEP	YEARLY	YEARLY	MONTHLY	YEARLY
COMPART. PRINT FREQ.	5	10	5	6
TIME SERIES VARIABLES	7	TDST	SPST	7
TIME SERIES/CUMULATIVE	TS/CUM	TS	TS	TS/CUM
OBSERVATION DEPTH	0.0	50	49	40
NUMBER OF HORIZONS	3	6	6	6
DEPTH TO WATER TABLE	2.5 m	5.0 m	5.0 m	4.2 m
EROSIONAL LOSSES	YES	YES	NO	NO
INITIAL PEST. RESIDUES	NO	NO	YES	NO
SOIL HYDRAULICS	RESTRICTED	FREE	FREE	FREE
NUMBER OF CROPS	1	3	3	3
PESTICIDE UPTAKE	NO	NO	NO	YES
INITIAL CROP No.	1	1	1	3
INITIAL CROP CONDITION	FALLOW	CROPPING	RESIDUE	FALLOW
COND. AFTER HARVEST	FALLOW	CROPPING	RESIDUE	RESIDUE
CROPPING PERIODS	3	20	3	5
CLIMATE DATA	ACTUAL	ACTUAL	20 YR MED.	ACTUAL
CLIMATE CHANGE	NO CHANGE	NO CHANGE	NO CHANGE	NO CHANGE

3.2 VERIFICATION OF THE LEACHM MODEL

Five tests were performed with both the modified and original versions of the LEACHM model to verify that the modified version of LEACHM, incorporated in the EXPRES expert system, is operating correctly. The five tests were designed to ensure that:

(1) the recompilation of the LEACHM program with the Microsoft® FORTRAN (v5.0) compiler was correct;

(2) the modified input data set was being read correctly;

(3) the modified meteorological data file was being read correctly;

(4) the snowmelt and pan evaporation calculations were accurate;

(5) the surface runoff and erosion calculations were accurate.

3.2.1 LEACHM TEST 1 - RECOMPILATION OF THE LEACHM PROGRAM

In the following discussions the modified version of the LEACHM model, used within EXPRES, will be referred to as LEACHMEX, while the original version of the model will continue to be referred to as LEACHM. The first test with the two LEACHM models was designed to verify the recompiled versions of both LEACHM and LEACHMEX with the Microsoft® FORTRAN v5.0 compiler. The test was run in a similar manner as that described for the PRZM model (Section 3.1.1). The results produced for the sample problem with both LEACHM and LEACHMEX (when compiled with the Microsoft® FORTRAN v5.0) were identical to the output for the sample problem provided by the model distributors.

Both the LEACHMEX and LEACHM models were also compiled and linked with the LAHEY® FORTRAN F77L-EM/32 compiler to test for additional errors or warning messages that would be produced by the LAHEY compiler. Several warning messages were produced with the LAHEY compiler for both the original (LEACHM) and modified (LEACHMEX) versions of the LEACHM model. Upon investigation of these warning messages a few errors were detected in the LEACHM models. Most of the errors were minor and did not significantly change the results produced by the models. However, the following error detected in the original (LEACHM) version of the model was significant.

The LEACHM model has four options for the bottom boundary condition in the simulation. The four options are:

(1) a constant potential - used when it is desired to simulate a water table within the simulated column;

(2) a free-draining profile - used when the water table is set below the bottom of the simulated soil column. A unit hydraulic gradient is assigned to the lowest node;

(3) zero flux past the lowest node - used for example if it is desired to simulate a perched water table;

(4) a lysimeter tank - used when simulating conditions approximated by a lysimeter tank. In this case, water drains from the column when the bottom node is saturated but has a zero flux when the bottom node is unsaturated.

The variable that held the value of the potential at the bottom of the simulated column when a water table or lysimeter was being simulated (options 1 and 4, respectively), was not being passed correctly from one subroutine to another because the common statements used to pass the value of the variable were not consistent. When this error was corrected, and the original version of the model was executed, the results produced were not meaningful. As a result these two options will be excluded in the modified version (LEACHMEX) of LEACHM that is incorporated in the EXPRES expert system. The user will be limited within EXPRES to simulating a free draining profile, or one with no flux past the bottom boundary. The authors of the LEACHM model will be notified of the errors in the original program, and if a solution to the difficulties with the bottom boundary potential is found, the water table and lysimeter tank options may be reintroduced into EXPRES, if time permits. Thus, this stage of the verification indicated that the two options discussed above can not be simulated with the LEACHMEX model.

3.2.2 LEACHM TEST 2 - VERIFICATION OF THE INPUT DATA SET

Eight simulations were performed in the second verification test of the two LEACHM models (four with LEACHM, and four with LEACHMEX). The objective of this test was to ensure that the common input data set was being read correctly by the modified input statements in the LEACHMEX model, and that all the possible options available in the LEACHMEX model were being read and executed correctly (similar to Section 3.1.2). Input data sets for both LEACHM and LEACHMEX were generated, and the results of the simulations with the two versions of LEACHM were compared to ensure that the options had been read and executed correctly by LEACHMEX. The results of the test indicate that the modifications made to the LEACHMEX model do not change the calculations of the model.

In a similar manner as that described for PRZMEX, all options in the LEACHMEX model were tested. Table 2 displays the pertinent values of the model parameters used in these simulations. There are four columns in Table 2 listing the model parameters used in the four simulations pairs. The same model parameter values were used in both the LEACHMEX and LEACHM simulations. In all cases, results produced by LEACHMEX were the same as those produced by LEACHM. Therefore, the operation of the modified version of LEACHM (LEACHMEX) is correct.

3.2.3 LEACHM TEST 3 - VERIFICATION OF THE METEOROLOGICAL DATA

In the third test performed, the accuracy with which the LEACHMEX version of the model reads the common meteorological data files was tested. Six simulations were performed for this test (three with LEACHMEX, and three with LEACHM). The three sets of simulations correspond to three sets of meteorological data, (1) the meteorological data file supplied with the original sample problem, (2) the actual data from the Charlottetown, PEI CDA weather station, and (3) median meteorological data for the Charlottetown, PEI CDA weather station. No errors were detected in reading these data files, and in all three pairs of simulations, the results produced by LEACHMEX were in agreement with those

Table 2. Model parameter data for the LEACHM verification tests.

LEACHM VERIFICATION				
	SIMULATION 1	SIMULATION 2	SIMULATION 3	SIMULATION 4
FILE NAME	TESTNEW1	TESTNEW2	TESTNEW3	TESTNEW4
STARTING DATE	010170	010170	010870	010170
ENDING DATE	311270	311270	311070	311270
NUMBER OF PESTICIDES	4	4	3	4
PARENT/DAUGHTER PRODUCTS	4-P,0-D	2-P,2-D	1-P,2-D	3-P,1-D
NO. OF PEST. APPLICATION	4	6	4	6
NO. OF PEST. APPLIED	4	4	3	4
DEPTH OF INCORP.	0.0 cm	10.0 cm	0.0 cm	10.0 cm
INITIAL PEST. RESIDUES	YES	NO	YES	NO
OUTPUT UNITS	µg/kg	µg/kg	µg/kg	mg/m^2
CONSTANT INTERVAL PRINT	30 DAYS	30 DAYS	5 DAYS	NO
PRINT ON SPECIFIC DAYS	NO	NO	NO	2 PRINTS
SUMMARY PRINT FREQUENCY	5 DAYS	7 DAYS	10 DAYS	7 DAYS
COMPARTMENT PRINT FREQ.	1	1	5	1
COMPARTMENT THICKNESS	100 mm	100 mm	150 mm	100 mm
NO. OF TIME SERIES FILES	4	4	4	2
PLANT OUTPUT TABLE	YES	YES	YES	NO
NUMBER OF HORIZONS	10	7	10	7
PROFILE DEPTH	1.1 m	2.5 m	3.0 m	2.5 m
DEPTH TO WATER TABLE	1.1 m	2.5 m	3.0 m	2.5 m
BOTTOM BOUNDARY COND.	FREE	FREE	ZERO FLUX	FREE
EROSIONAL LOSSES	NO	NO	NO	NO
NUMBER OF CROPS	5	1	2	2
CROPPING PERIODS	5	1	2	2
PLANTS PRESENT	YES	YES	YES	YES
PLANT ROOTS	CONSTANT	CONSTANT	GROWING	CONSTANT
PESTICIDE UPTAKE	NO	YES	NO	NO

produced by LEACHM. Thus, it can be concluded that the LEACHMEX version of the LEACHM model correctly reads the meteorological data.

3.2.4 LEACHM TEST 4 - VERIFICATION OF THE SNOWMELT AND PAN EVAPORATION CALCULATIONS

The snowmelt and pan evaporation estimation routines added to the modified LEACHM model (LEACHMEX) are identical to those used in the original PRZM model. Therefore, the additions to the LEACHM model were verified by comparing the amount of snowmelt and pan evaporation calculated in the LEACHMEX model with the results of similar calculations made by the original PRZM model. Figure 1 indicates that the LEACHMEX model calculations for snowmelt and pan evaporation are the same as those in the PRZM model. Because these processes have been tested and verified by the developers of the original PRZM model and others (Carsel et al., 1984;1985, Jones, 1985;1986, Jones et al., 1986, and Pennell et al., 1989), it is conclude that the snowmelt and pan evaporation calculations in the LEACHMEX model are accurate.

3.2.5 LEACHM TEST 5 - VERIFICATION OF THE SURFACE RUNOFF AND EROSION SUBROUTINE

The runoff and erosion subroutine added to the modified LEACHM model (LEACHMEX) are also based on runoff and erosion subroutines in the original PRZM model. Verifications tests were therefore performed, by comparing the amount of water and pesticide lost by runoff and erosion predicted by LEACHMEX, with the predicted loss as calculated by the original PRZM model. However, unlike the snowmelt and pan evaporation routines, which depend only on the climatological data entered and are independent of the rest of the model, the runoff and erosion routines depend on the water content and pesticide concentration found in the surface layers of the soil. Therefore, the runoff and erosion calculations are dependent on the manner in which water and solutes are transported through the soil profile. The LEACHMEX and PRZM models take different

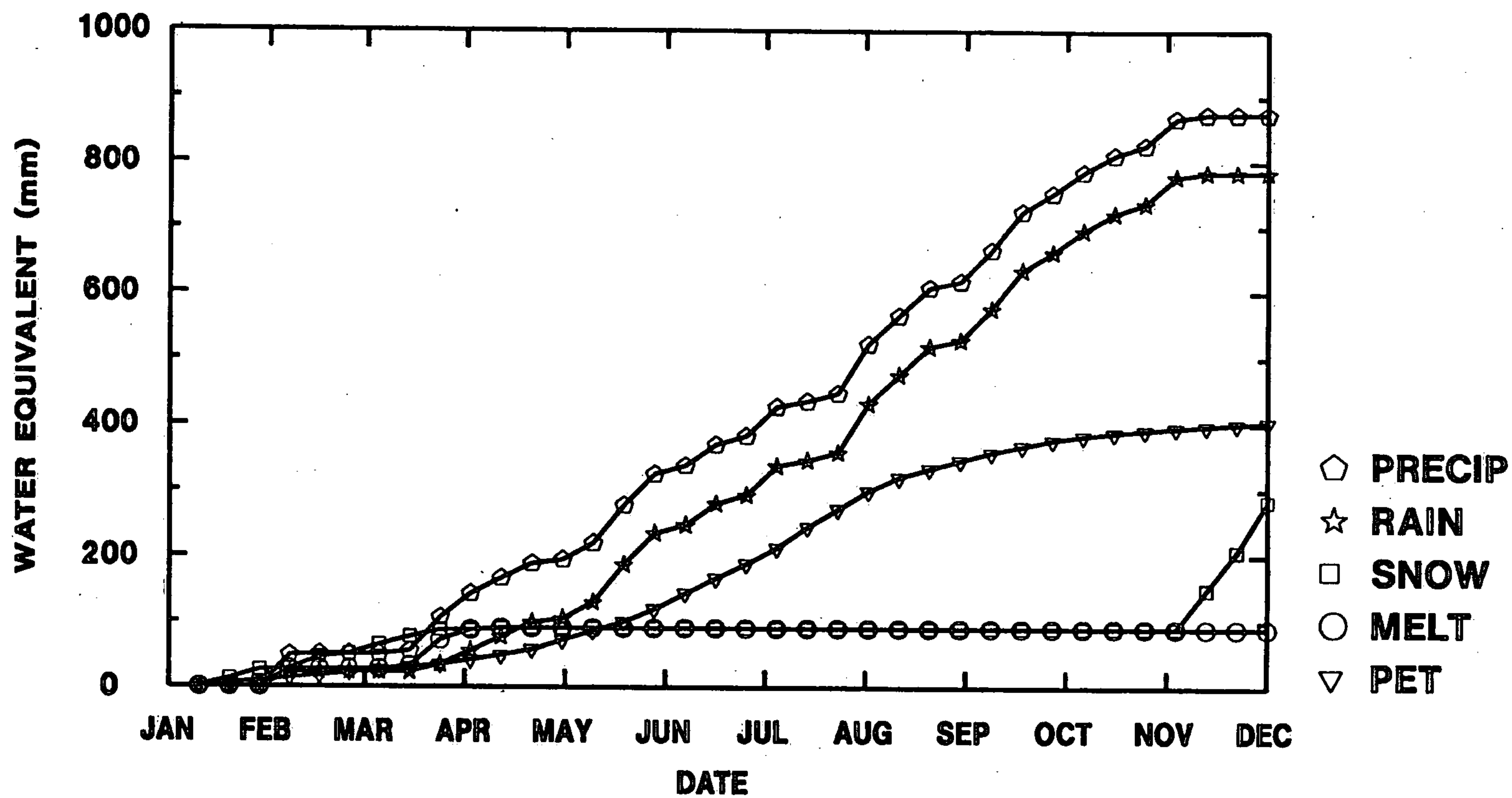

Figure 1. Comparison of snowmelt and pan evaporation estimates made by PRZM and LEACHMEX. Data represents cumulative total over a one year time span. The solid lines represent LEACHM predictions. Symbols represent PRZM predictions

approaches to the routing of water and pesticide in the soil profile. The LEACHMEX model attempts to describe the actual processes involved in the flow of water in the unsaturated zone, while the PRZM model uses a simplified water flow representation based on two soil parameters. The reader is referred to the Phase 1 Report (Mutch and Crowe, 1990) for further details on the different water flow representations used in the two models. Because of the differences in the water flow representations in the two models (PRZM and LEACHMEX), the calculations for the loss of water and pesticide via runoff and erosion in the two models will not be identical. As a result, the loss of water and pesticide via runoff and erosion predicted by the two models was compared for 3 - one year simulations. The results are presented in Figures 2 through 4, and indicate that the amount of surface runoff and erosion losses predicted by the LEACHMEX model are in excellent agreement with the results predicted by the original version of the PRZM model. Although the LEACHMEX model may not predict identical amounts of surface runoff and erosion as that predicted by the PRZM model, Figures 2 - 4 show that over the period of a one year simulation, the cumulative amounts of surface runoff and erosion are similar, and following the reasoning used in Section 3.2.4, it can be concluded that the surface runoff and erosion routines added to the LEACHMEX model are accurate.

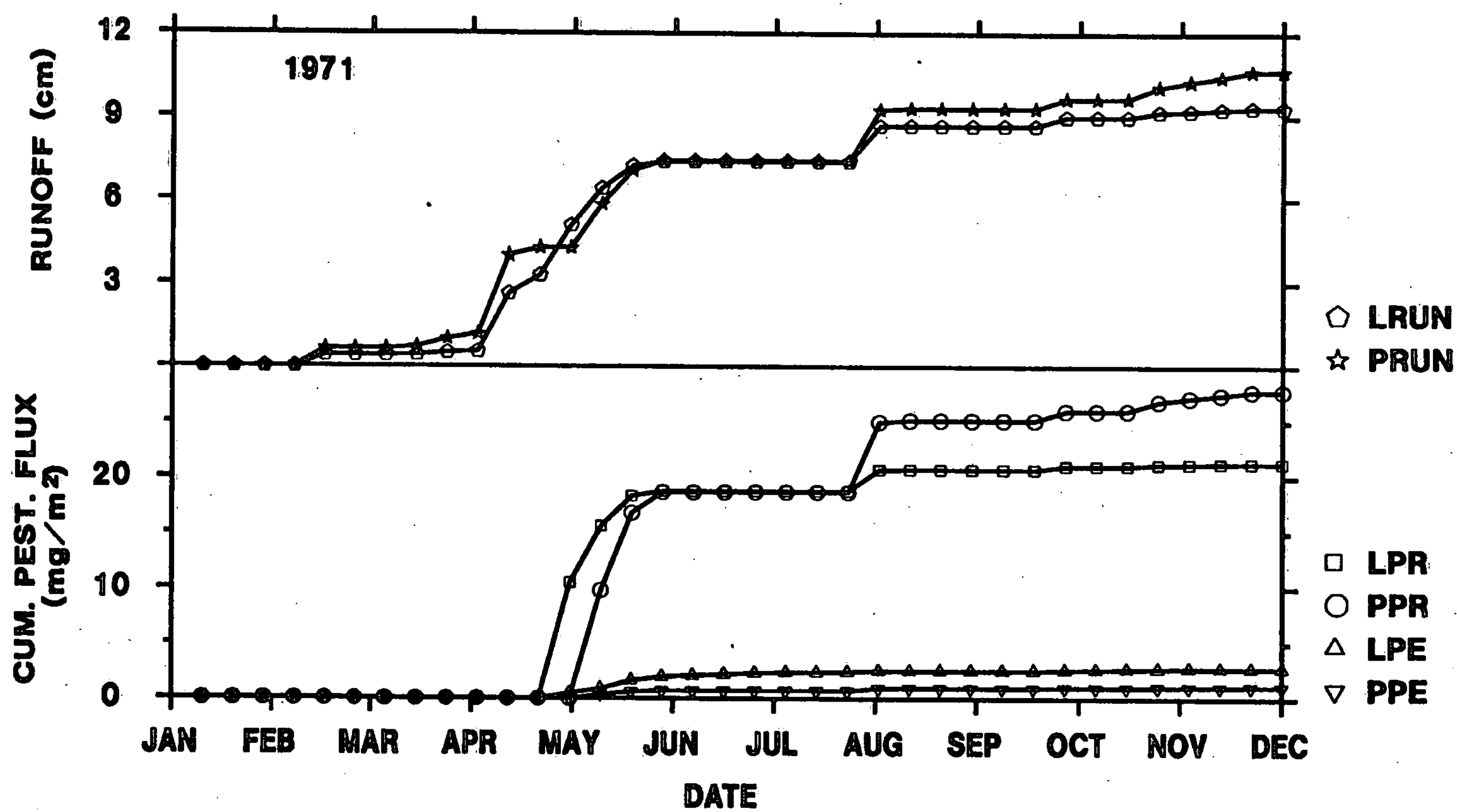

Figure 2. Comparison of runoff and erosion results predicted by PRZM and LEACHMEX. (1971) LRUN - cumulative runoff depth (LEACHMEX), PRUN - cumulative runoff depth (PRZM), LPR - cumulative pesticide flux loss in runoff (LEACHMEX), PPR cumulative pesticide flux loss in runoff (PRZM), LPE - cumulative pesticide flux loss by erosion (LEACHMEX), PPE - cumulative pesticide flux loss by erosion (PRZM).

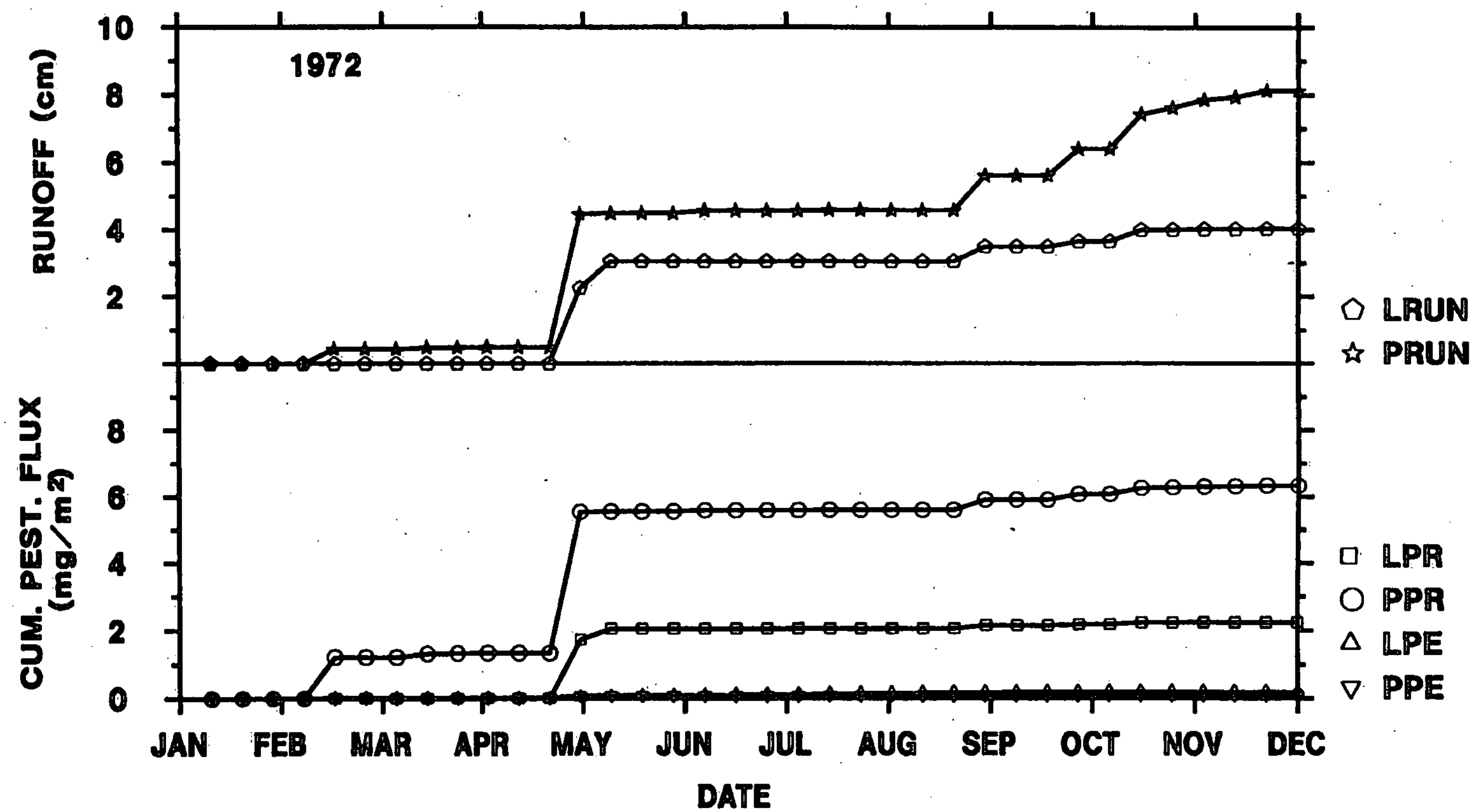

Figure 3. Comparison of runoff and erosion results predicted by PRZM and LEACHMEX. (1972) LRUN - cumulative runoff depth (LEACHMEX), PRUN - cumulative runoff depth (PRZM), LPR - cumulative pesticide flux loss in runoff (LEACHMEX), PPR cumulative pesticide flux loss in runoff (PRZM), LPE - cumulative pesticide flux loss by erosion (LEACHMEX), PPE - cumulative pesticide flux loss by erosion (PRZM).

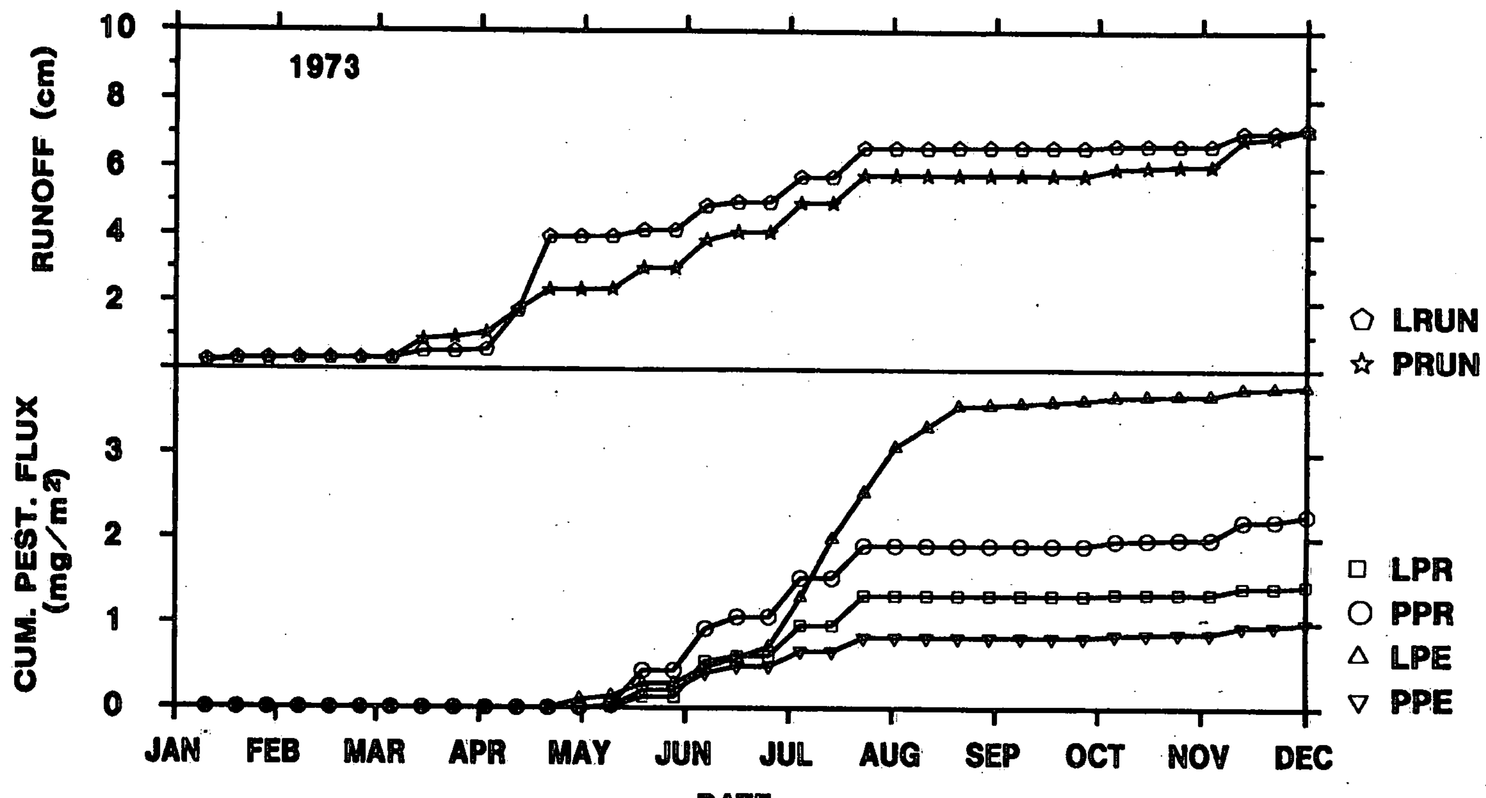

Figure 4. Comparison of runoff and erosion results predicted by PRZM and LEACHMEX. (1973) LRUN - cumulative runoff depth (LEACHMEX), PRUN - cumulative runoff depth (PRZM), LPR - cumulative pesticide flux loss in runoff (LEACHMEX), PPR cumulative pesticide flux loss in runoff (PRZM), LPE – cumulative pesticide flux loss by erosion (LEACHMEX), PPE - cumulative pesticide flux loss by erosion (PRZM).

4.0 CONCLUSION

Two types of tests were conducted with the modified versions of the two models (PRZMEX and LEACHMEX) to ensure that the modifications made to the models did not disrupt the validity or accuracy of the calculations performed by the two models. Firstly, where appropriate, the results of simulations undertaken with the modified versions of either LEACHM or PRZM (LEACHMEX or PRZMEX, respectively) were compared to the results from the original versions of LEACHM and PRZM. Secondly, because additional processes were added in the modifications made to the LEACHM model, simulations with the additional processes in place could not be compared to the original code. Hence, verification was undertaken by comparing the results obtained using the modified version of the LEACHM model (LEACHMEX) to the results obtained from the original PRZM model, on which the modifications to LEACHM were based.

The dialogue format of the expert system was verified by performing a sufficient number of simulation to test all options available in the two models. In all of the test simulations, the options were read and executed correctly by EXPRES.

The physical and chemical processes added to the LEACHMEX model (snowmelt, pan evaporation estimation, surface runoff and erosion) were similar to processes simulated in the original PRZM program, and the modifications in the LEACHMEX model were verified by comparing the results calculated for the additional processes with the results from the original PRZM model which has previously been verified. The results for the snowmelt and pan evaporation estimation were identical to the results produced by the original version of the PRZM model. The estimation of surface runoff and erosion depends on the water content and pesticide concentrations in the surface layers of the soil, and therefore, the amount of surface runoff and erosion will depend on the approach taken in simulating water and pesticide transport in the unsaturated zone. The PRZM and LEACHMEX models take different approaches in simulating water and pesticide transport, so they will not predict identical amounts of surface runoff and erosion. However, the results of 3 one-year simulations indicate that there is a excellent agreement between the amount of runoff and erosion predicted by the two models over this time frame.

The verification tests that have been described in this report all indicate that the modified versions of the LEACHM and PRZM models are producing results that, where appropriate, are (1) consistent with the original versions of the models, (2) accurately simulating the new processes added to the models, and (3) indicate that the interface between the two models and the EXPRES expert system is functioning correctly.

5.0 REFERENCE LIST

Carsel, R.F., Smith, C.N., Mulkey, L.A., Dean, J.D., and Jowise, P., 1984. User's manual for the pesticide root zone model (PRZM), release 1. EPA-600/3-84-109, US Environmental Protection Agency, Athens, GA, 216 p.

Carsel, R.F., Mulkey, L.A., Lorber, M.N., Baskin, L.B., 1985. The Pesticide Root Zone Model (PRZM): A procedure for evaluating pesticide leaching threats to groundwater. Ecological Modelling, Vol. 30, pp. 49-69.

Climatological Services Division, 1990. Meteorological data for the Charlottetown, PEI CDA weather station. Climatological Services Division, Climatological Applications Branch, Canada Climate Centre, 4905 Dufferin Street, Downsview, Ontario, M3H 5T4.

Haith, D.A. and Loehr, R.C., (Eds.), 1979. Effectiveness of soil and water conservation practices for pollution control. U.S. Environmental Protection Agency, Athens, Georgia, Report No. EPA-600/3-79-106.

Jones, R.L., 1985. Effect of application methods on movement and degradation of aldicarb in Maine potato fields. Environmental Toxicology and Chemistry, 5:167-173.

Jones, R.L., 1986. Field, laboratory, and modelling studies on the degradation and transport of aldicarb residues in soil and groundwater. In: W.Y.Garner, R.C.Honeycutt and H.N.Nigg (Editors), ACS Symposium Series - Evaluation of Pesticides in Ground Water. American Chemical Society, Washington,D.C., 315(11), pp. 197-218.

Jones, R.L., Black, G.W., and Estes, T.L., 1986. Comparison of computer model predictions with unsaturated zone field data for aldicarb and aldoxycarb. Environmental Toxicology and Chemistry, Vol. 5, pp. 1027-1037.

Mutch J.P. and Crowe A.S., 1990. An expert system for assessing the migration and transformation of pesticides in the subsurface; Phase 2 report: Development of the basic expert system. Submitted as a National Water Research Institute manuscript, Environment Canada, 48 pp.

Mutch, J.P. and Crowe, A.S., 1989. An expert system for assessing the migration and transformation of pesticides in the subsurface; Phase 1 report: A review and analysis of existing pesticide transport models. National Water Research Institute manuscript, NWRI #89-172, Environment Canada. 36 pp.

Pennell, K.D., Hornsby, A.G., Jessup, R.E., and Rao, P.S.C., 1989. Evaluation of five simulation models for predicting aldicarb and bromide behaviour under field conditions. In preparation for Water Resources Research, November 6, 1989 draft.

Wagenet, R.J. and Hutson, J.L., 1986. Predicting the fate of nonvolatile pesticides in the unsaturated zone. Journal of Environmental Quality, 15(4):315-322.

Wagenet, R.J., and Hutson, J.L., 1987. LEACHM: Leaching Estimation And CHemistry Model. Water Resources Institute Continuum, Center for Environmental Research, Cornell University, Ithaca, New York, Volume 2, 80 p.

Williams, J.R. and Brendt, H.D., 1977. Sediment yield prediction based on watershed hydrology. Trans. ASAE, 20:1100-1104.

NATIONAL WATER RESEARCH INSTITUTE
P.O. BOX 5050, BURLINGTON, ONTARIO L7R 4A6

Environment Canada Environnement Canada

Canada

INSTITUT NATIONAL DE RECHERCHE SUR LES EAUX
C.P. 5050, BURLINGTON (ONTARIO) L7R 4A6